

Quantum Phase Transition in Dimerized Spin-1/2 Chains

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Abstract

Quantum phase transition in dimerized antiferromagnetic Heisenberg spin chain has been studied. A staircase structure in the variation of concurrence within strongly coupled pairs with that of external magnetic field has been observed indicating multiple critical points. Emergence of entanglement due to external magnetic field or magnetic entanglement is observed for weakly coupled spin pairs in the same dimer chain. Though closed dimerized isotropic XXX Heisenberg chains with different dimer strengths were mainly explored, analogous studies on open chains as well as closed anisotropic (XX interaction) chains with tilted external magnetic field have also been studied.

1 Introduction

Quantum phase transition (QPT) is a phenomenon where the non-analyticity in the energy level gives rise to a situation where energy fluctuation at the critical point vanishes [1]. Entanglement in a quantum system may be considered as a witness of this phenomenon (see e.g. [2,3]). On the other hand, entanglement being an important resource [4–7] in quantum information processing, this phenomenon is important from the perspective of its physical realization too.

Spin-1/2 chains are some of the simplest qubit systems considered in the literature (see e.g. [8–11]) for the implementation quantum processor. Again the case of a two spin system, interacting through an isotropic XXX Heisenberg Hamiltonian in presence of an external magnetic field, the entanglement of formation has been calculated by Nielsen [12], which was further extended for a spin chain under periodic boundary conditions with a systematic investigations on the variation of entanglement between various sites due to that of an external magnetic field and temperature (see [2]). The pairwise entanglement vanishes even at a vanishingly small temperature if the magnetic field exceeds a critical value which characterises quantum phase transition. The effect of magnetic entanglement on isotropic XY model and thermal entanglement for anisotropic XY model [13] and with non zero external magnetic field the effect of anisotropy on the same system had also been studied [14]. The dynamical phase transition in anisotropic XY model was also been studied [15].

The effect of non uniform magnetic field on thermal entanglement for the two qubit system with isotropic Heisenberg interaction [16] and for a two-qubit Ising model [17] were studied. Gong and Su [18] have investigated pairwise thermal entanglement in $S = \frac{1}{2}XY$ chain (including

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its thermodynamic limit $N \rightarrow \infty$) and compared their results, with mean field frame work. They have found that in the case of first model there exist a common T_c , independent of B for both ferromagnetic and anti-ferromagnetic interactions. It had also been found that in such a spin system T_C is independent of B for AF interactions. The studies were further extended for Heisenberg model with next to nearest neighbour interaction [19] and existence of two types of QPT was noticed. Other possibilities like existence of tilted external field [20], mixed chain with spin-1/2 and spin-1 elements [21], were also explored. Far from equilibrium QPT has been observed in an open Heisenberg XY spin- $\frac{1}{2}$ chain characterized by a sudden appearance of long-range magnetic order in the non-equilibrium steady state as the magnetic field is reduced [22]. In fact for last one and half decade or so, QPT in Ising chains and Heisenberg chains was extensively studied by different workers, only some of which we mentioned here.

Though the dimerized versions of Heisenberg spin chains were studied since a long time back, they got renewed interests from the perspective of quantum communication. On the other hand, for quite a long time spin chains are proposed candidates for communication medium between two quantum processors (see e.g. [23] and references therein). But very recently a scheme of information transfer has been proposed [24] using dimerized spin-1/2 XXX model. Another scheme to generate end to end entanglement has also been proposed [25] using dimerized XXX and XXZ model. Although phase transition in dimerized spin-1/2 chain was studied in connection with transition between gapped and ungapped energy spectra (see e.g. [26, 27]), quantum phase transition for the dimerized cases using thermal and magnetic entanglement has not been studied yet according to the authors' knowledge. The present paper explores this field for spin-1/2 dimerized Heisenberg chain.

2 Formalism

The exchange Hamiltonian of a Heisenberg spin chain may be generalised as

$$H_E = \sum_i (J_x \sigma_i^x \sigma_{i+1}^x + J_y \sigma_i^y \sigma_{i+1}^y + J_z \sigma_i^z \sigma_{i+1}^z), \quad (1)$$

where J_x , J_y and J_z are the coupling strengths along three orthogonal directions. In addition if some external magnetic field \vec{B} is applied on the system, there will be additional on-site energy terms, generally called as Zeeman energy terms, as

$$H_B = \sum_i \vec{B} \cdot \vec{\sigma}_i. \quad (2)$$

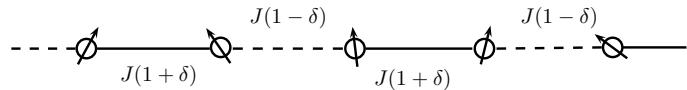


Figure 1: Schematic diagram of a dimer chain

The dimerized Hamiltonian for a chain of N spins in presence of an external uniform magnetic field acting along z -axis is given by

$$H = B \sum_{i=1}^N \sigma_i^z + J \sum_{i=1}^N [1 + (-1)^{i+1} \delta] \vec{\sigma}_i \cdot \vec{\sigma}_{i+1} \quad (3)$$

where

$$\vec{\sigma}_i = (\sigma_i^x, \sigma_i^y, \sigma_i^z)$$

are the Pauli spin matrices and the dimer strength is denoted by δ ; with $0 \leq \delta \leq 1$. It is quite obvious from the expression that the coupling strength becomes strong and weak alternately for consecutive pairs which characterises a dimer. For the AFM chains the interaction strength $J > 0$ and for the FM cases $J < 0$. For a closed chain i runs from 1 to N in the second summation within the Hamiltonian expression, eq. (3), with the boundary condition $\vec{\sigma}_{N+1} \equiv \vec{\sigma}_1$; while for open chain i simply runs from 1 to $N - 1$. For an external magnetic field tilted by an angle θ with z -axis, eq. (3) may be modified as

$$H = B \cos \theta \sum_{i=1}^N \sigma_i^z + B \sin \theta \sum_{i=1}^N \sigma_i^x + J \sum_{i=1}^N [1 + (-1)^{i+1} \delta] \vec{\sigma}_i \cdot \vec{\sigma}_{i+1}. \quad (4)$$

The system is taken to be in thermal state i.e., the state of the system when it is at thermal equilibrium with a thermal bath (environment) at temperature T , such that the density matrix, $\rho(T) = \exp(-\frac{H}{kT})/Z$ where Z is the partition function and k is Boltzman's constant. In this communication we are reporting the variation of pairwise thermal entanglement for the strongly coupled and weakly coupled spin pairs separately with that of magnetic field as well as that of dimer strength δ for a closed AFM chain(along with the open ended ones) of length N .

For this purpose first we need to find out the pairwise entanglement of qubit pairs. This may be obtained from the reduced density matrix for that pair of qubit, evaluated by tracing out the contribution of other qubits (or in other words taking partial trace on those degrees of freedom) from the total density matrix $\rho(T)$ of the system. Thus the reduced density matrix of the subsystem (spin pair) of our concern may be expressed as

$$\rho_R = \text{Tr}_B [\rho(T)],$$

where the complementary part of the system is named as subsystem B.

Now in general ρ_R will be of mixed state. For such a system the suitable measure of entanglement may be considered as entanglement of formation which may be expressed, for a two qubit system, as a monotonic function of a simpler variable named as concurrence [28]. From reduced density matrix the following product matrix was calculated

$$R = \rho_R (\sigma_y \otimes \sigma_y) \rho_R^* (\sigma_y \otimes \sigma_y) \quad (5)$$

If we represent λ_i 's with $i = 1, 2, 3, 4$ as the square root of the eigenvalues of R in descending order then concurrence can be expressed as

$$C = \max(0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4) \quad (6)$$

In this method we have described the standard bases, $|00\rangle, |01\rangle, |10\rangle, |11\rangle$ must be used. In this study we have calculated the concurrence indicating the thermal entanglement between different spin pairs.

3 Multiple Transitions and Staircase Structure

Following the same line of investigation as done in the ref. [2], we investigated the pairwise entanglement of nearest neighbour pairs for a closed chain as quantified by the concurrence; but in this case for two types of pairs viz., strongly coupled and weakly coupled separately.

It is quite apparent, from the figures 2 and 3, that in the case of a dimer too, there is a sharp critical value of $B = B_c$ across which the pairwise entanglement, both in the case of strongly coupled as well as of weakly coupled pairs abruptly vanishes. At very low temperatures the it is more abrupt due to the minimal presence of thermal fluctuations indicating some quantum

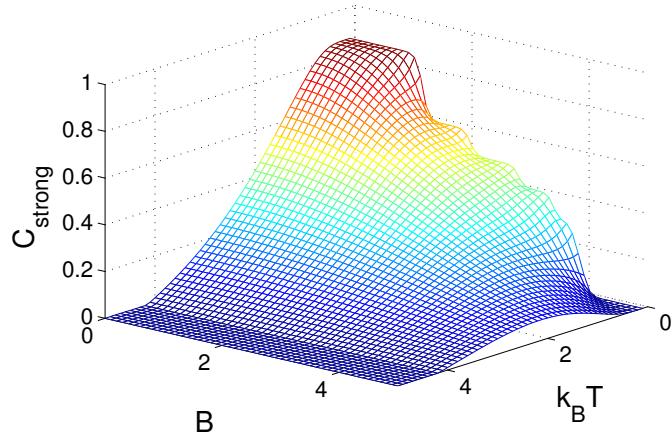


Figure 2: Variation of entanglement between strongly coupled spin pairs with temperature and external magnetic field for closed XXX chain. $N = 12, \delta = 0.2, \theta = 0$

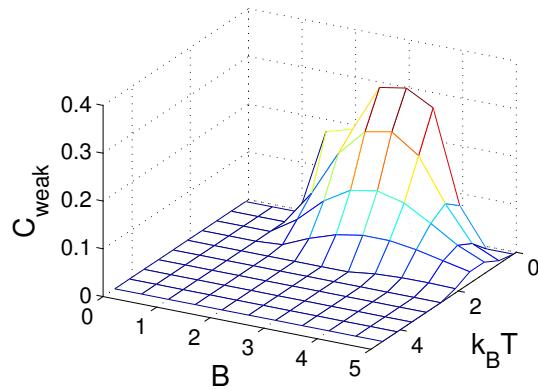


Figure 3: Variation of entanglement between weakly coupled spin pairs with temperature and external magnetic field for closed XXX chain. $N = 12, \delta = 0.2, \theta = 0$.

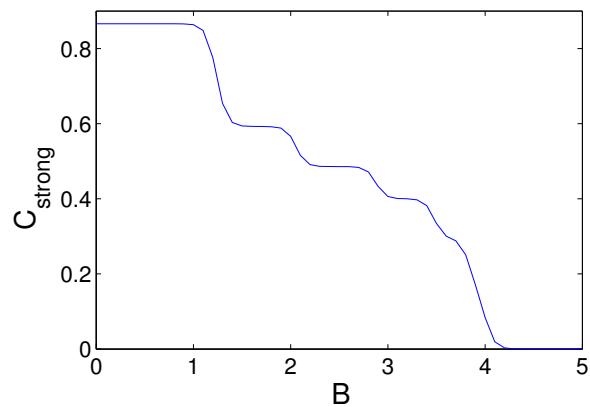


Figure 4: Variation of entanglement within strongly coupled pair with magnetic field at constant temperature i.e with fixed $k_B T = 0.1$. $N = 12, \delta = 0.2, \theta = 0$.

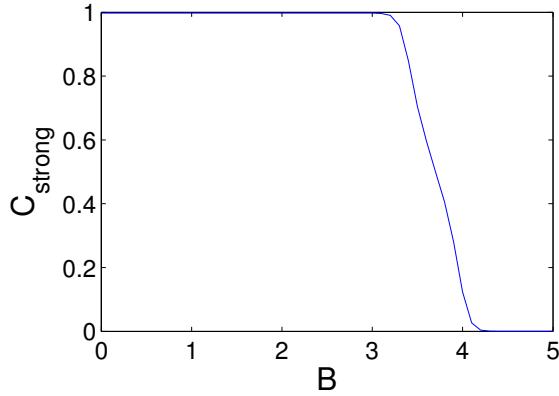


Figure 5: Variation of entanglement within strongly coupled pair with magnetic field at constant temperature i.e with fixed $k_B T = 0.1$. $N = 12, \delta = 0.8, \theta = 0$.

phase transition at this value of B . The transition becomes progressively blurred at higher temperatures and ultimately vanishes at a critical temperature $T = T_c$ above which thermal fluctuations dominate destroying all pairwise entanglement in the chain. But apart from these features also available in the non-dimerized version of Heisenberg chain as observed by several authors, there are certain distinctive characteristics available for the case of its dimerized version. First of all the values of concurrences in strongly coupled pairs are almost maximal (> 0.9) while it is zero for weakly coupled pairs even for $\delta = 0.2$ (see figs. 2 & 3) in absence of any external magnetic field. Moreover particularly at low temperatures, there exist certain other discrete values of B , for each of which the pairwise concurrence for the strongly coupled pairs abruptly diminishes to a lower value and then remains steady with the increase of B , until next such critical value of B arrives; giving rise to a staircase structure (see fig. 2), which is easier to identify when one takes a constant temperature 2-d slice at a low temperature like the figure 4 and 5. It may be apparent from these figures (figs. 4 and 5) that this staircase structure is more pronounced with smaller values of dimer strength δ .

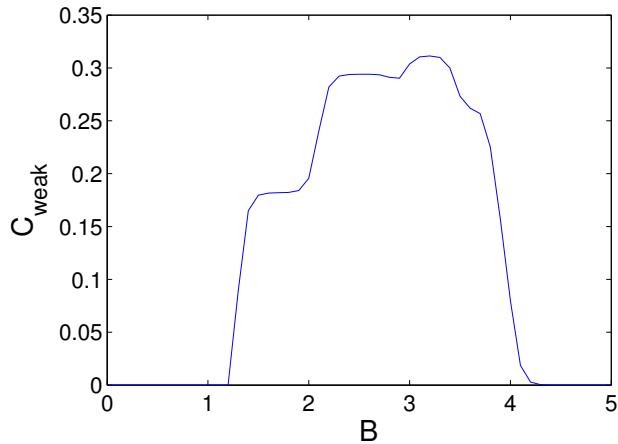


Figure 6: Variation of entanglement within weakly coupled pair with magnetic field at constant temperature i.e with fixed $k_B T = 0.1$. $N = 12, \delta = 0.2, \theta = 0$.

The same observations for weakly coupled pairs of the same chain (fig. 3) also revealed such

staircase structure (particularly with small δ , as in fig. 6) but that structure becomes blurred with higher values of δ , except a certain surge near the final B_c (see fig. 7). It may be noted that at the extreme value of $\delta = 1$, the weakly coupled pairs get decoupled and hence entanglement within those pairs vanishes at that limit. Moreover it is apparent from the figs. 6 & 7 that at zero magnetic field weakly coupled pairs are completely separable and they get entangled only after a specific value of external magnetic field sets in (depending upon δ), which may be considered as a case of magnetic entanglement.

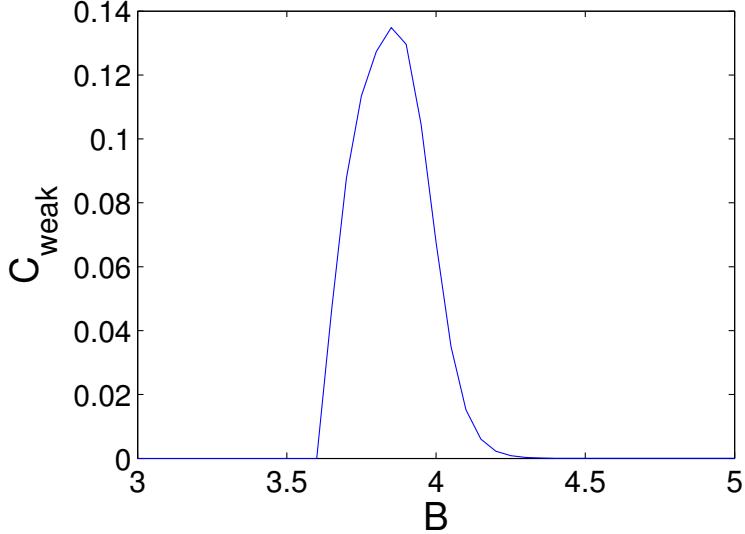


Figure 7: Variation of entanglement within weakly coupled pair with magnetic field at constant temperature i.e with fixed $k_B T = 0.1$. $N = 12, \delta = 0.8, \theta = 0$

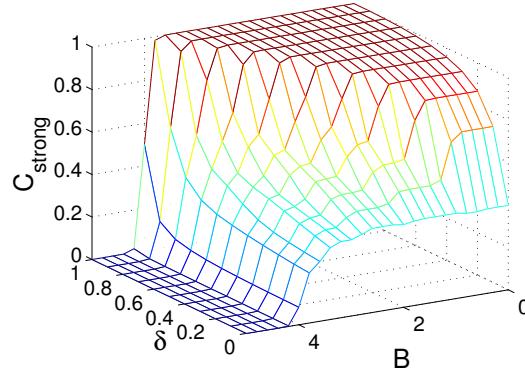


Figure 8: Variation of concurrence in strongly coupled pairs with the variation of B and δ at a fixed temperature $k_B T = 0.1$.

Next the variation of concurrence within strongly coupled pairs with that of external magnetic field and that of dimer strength (see fig.8) at a constant low value of temperature shows that this staircase feature is more predominant for relatively low values of dimer strengths.

From the 3-D plot (fig.'8) it is clear that, if δ increases from 0 even by a small amount (i.e. making it non-dimer chain) the staircase structure of the variation of concurrence with external

magnetic field appears and the stair sizes vary with δ and it vanishes when δ approaches the value 1, the limit in which the chain breaks into a collection of identical spin pairs interacting with XXX Hamiltonian.

The staircase structure may be contributed by the gapped nature of the energy spectra for dimer chains, but further investigation is required to identify the actual mechanism.

To investigate the effect of inclination of external magnetic field, the dimerized XX chain is chosen. The variation of the inclination of magnetic field has also been studied and for different angles the variations of the pairwise entanglement with field strength are plotted in figs. 9, 10 & 11. It has been found that for XX dimer chain even the strongly coupled pairs develop less amount of entanglement as expected intuitively, but it is observed that at low temperature with the increase of B , the entanglement first diminishes to almost zero at a critical value of B and then again build up; moreover this build up increases with the relative strength of the longitudinal component of external field, i.e. B_x or in other word with the angle of tilt. Similar secondary build up of entanglement was also reported by some authors earlier for two qubit anisotropic Heisenberg chain with the variation of anisotropy (see [3, 14]).

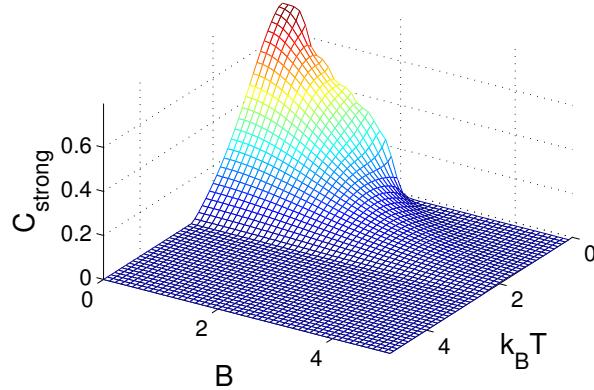


Figure 9: The variation of concurrence in strongly coupled pair [$\delta = 0.2$] in XX model with B and $k_B T$ for tilted B at an angle $\theta = 0$ with z -axis.

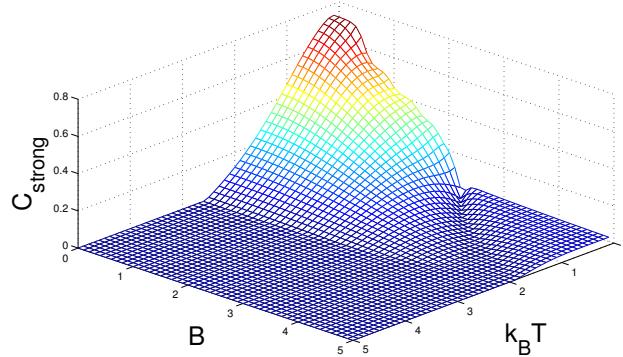


Figure 10: The variation of concurrence in strongly coupled pair [$\delta = 0.2$] in XX model with B and $k_B T$ for tilted B at an angle $\theta = \pi/4$ with z -axis.

The studies already mentioned correspond to closed chains which have translational symmetry. But as this study has been motivated by the communication aspect of the dimers as

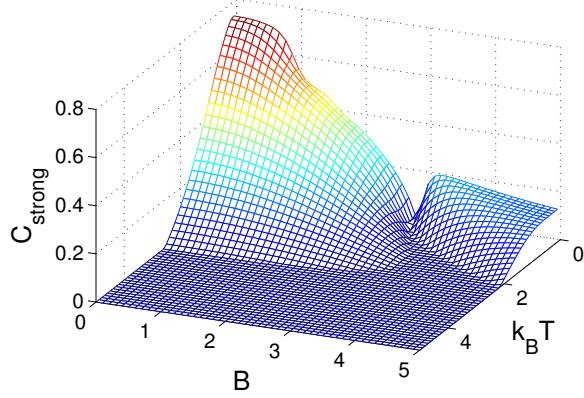


Figure 11: The variation of concurrence in strongly coupled pair [$\delta = 0.2$] in XX model with B and $k_B T$ for tilted B at an angle $\theta = \pi/2$ with z -axis i.e. along x -axis.

recently proposed by some authors (refs), it is natural to extend these studies for open XXX dimer chains. Due to absence of translational symmetry each pair has some unique feature in phase transition. We have chosen one strongly coupled one at the edge (fig. 12) and another one near the middle of the chain (fig. 13).

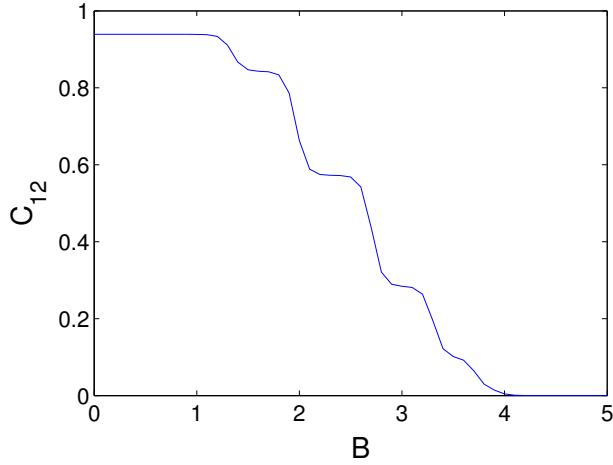


Figure 12: Variation of concurrence in the first strongly coupled pair of an open XXX chain with external magnetic field B for $\delta = 0.2, N = 12$

It is clearly seen that the staircase structure is retained for the open chains too and in absence of external field strongly coupled ones are almost maximally entangled. The pair at the edge almost replicates (fig. 12) the features corresponding to strongly coupled pairs in closed chains; but for the pair near the middle shows (fig. 13) a build up at some intermediate values of B , which is not found for strongly coupled pairs in closed XXX chains.

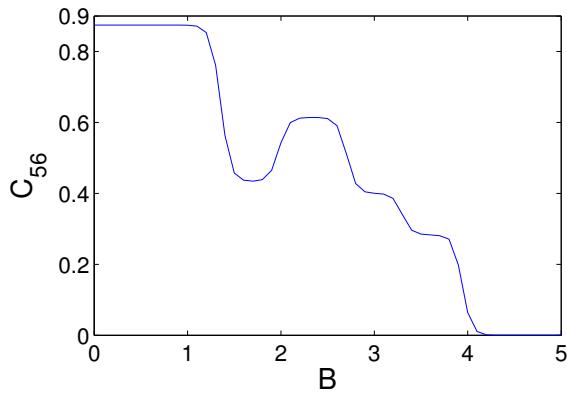


Figure 13: Variation of concurrence in the fifth pair (strongly coupled) of an open XXX chain with external magnetic field B for $\delta = 0.2, N = 12$

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